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Progress in the Parallelization of the SOCRATES-P Missile Plume Code

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Abstract

We report progress in the implementation of a parallelized version of SOCRATES under HPCMP CHSSI Project CFD-10. Examples of the increased capabilities of the Pre-Alpha code are given, along with an overview of the software design approach.

1. Introduction.

SOCRATES is the DoD standard high altitude missile plume code, designed to predict the optical properties of a multi-species, chemically reacting, non-equilibrium gas flowfield surrounding a missile in high altitude flight. It is based on the computationally-intensive, statistical Direct Simulation Monte Carlo method. The nominal code is serial and is written in structured fortran77. Current analysis requirements make it imperative to transition the code to a parallel environment, while the need to support continual evolution of the code requires development of a more modern, maintainable, and modular software package.

2. Objective.

The nominal parallelization plan includes consideration of two distinct paradigms: a distributed version, and also a conventional domain-decomposition approach. Code modernization is made possible by conversion to a more object-oriented and modular fortran90 approach. Additionally, the basic capabilities of the code are being improved.

3. Methodology.

The evolution of SOCRATES into SOCRATES-P involves the incremental replacement of datastructures, routines, and modules, along with the addition of new features. A working version of the nominal code is maintained at all times during the development.

4. Results.

The project will be undergoing Alpha test review during the third quarter of FY2003, with Beta test expected in FY2005. We present results for the scalability of the distributed version of the pre-alpha code on several HPC platforms, along with examples of the improved usability to appear in the code, such as automated volume grid-generation.

5. Significance.

The distributed parallel version of the Alpha code will be made available to interested users in FY2003. For a certain class of applications, this code will offer improved accuracy and computational efficiency, while retaining all features of the nominal, well-validated serial SOCRATES code currently available. The code will be hosted on a variety of HPC platforms. All versions of the code will be export-controlled.